

TRC Thermophysical Property Databases

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Thermochemical and thermophysical properties of the chemicals represent the numerical base for any commercial chemical engineering simulations. Over more than 55 years, Thermodynamics Research Center at Texas A&M University, one of the oldest and the most authoritative research centers in the world, has been involved in the collection, critical evaluation, and correlation of thermophysical and thermochemical data for organic compounds. Over the last 20 years a number of electronic databases for thermophysical properties was developed. These databases are widely used by the industry.

The operational structure and the scope of two major TRC databases (SOURCE and TABLE) will be discussed. TRC SOURCE database was developed and maintained over the period of 14 years and serves primarily as a major archive of original experimentally measured values of thermophysical and thermochemical data. It contains 112,000 Chemical Abstracts Service Registry Numbers along with information on molecular structure, chemical names and net formulas, 80,000 literature references and 800,000 property values and associated metadata covering 16,000 pure compounds, 10,000 binary and ternary mixtures, and 3,000 chemical reactions. The product is maintained in the form of an ORACLE 8 relational database, Enterprise Edition residing on a Digital Personal Workstation Alpha-series. Data screen and keyboard access is made by ORACLE Forms. Based on its long-term cooperation programs with a variety of research centers worldwide TRC has developed the standardized input data file formats and the batch entry subroutines. The options available for the remote data entry as well as the Internet distribution of the data will be demonstrated. TRC TABLE database is essentially an electronic version of TRC Tables-Hydrocarbons and TRC Tables-Non-Hydrocarbons published by TRC since 1952. It contains the recommended thermophysical properties for more than 7,600 compounds. Since each data point in the SOURCE database is characterized with the estimated uncertainty, the evaluation of the recommended data might be in principle produced 'to order'. That concept was used for the first time to develop a new product, DataExpert System, produced jointly by TRC and National Engineering Laboratory (NEL) in Glasgow (UK). This product is a combination of SOURCE and TABLE databases as well as LOADER-2 software developed at NEL. The DataExpert System will be demonstrated.

TRC PC-databases for various thermophysical properties of pure organic compounds and their mixtures (Vapor Pressure Database, Ideal Gas Properties Databases, COMPOUNDS Database, Floppy Book package) will be demonstrated.